Monte Carlo Simulation of Electron Transport Coefficients in Oxygen, Nitrogen, and Air

Mohammed Habib Allah Lahouel[1], Djilali Benyoucef [*1], Hocine Tebani [1]

Laboratoire Génie Electrique et Energies Renouvelables, Chlef University, Algeria

* d.benyoucef@univ-chlef.dz

The electrical discharges in air are a technology of great interest for certain environmental-related industrial sectors such as water treatment and air sterilization by ozone generators or the depollution by precipitators, when it comes to the removal of industrial particles, dust and/or heavy metals; or by corona discharge reactors with or without DBD depending on the geometries of the electrodes [1,2,3]. The modeling makes it possible to optimize these electric discharges through the knowledge of the physical and chemical phenomena intervening in the discharge dynamic. Generally the model used at atmospheric pressure is the fluid model, the latter is based on the first moments of the Boltzmann equation and requires some average quantities called transport coefficients.

The main objective of this work is the calculation of the electron transport coefficients in oxygen, nitrogen, and air. They are calculated by using Monte Carlo method [4,5], and the results obtained are compared to the measurements in order to validate the used data for each gas.

Key words: Monte Carlo Method, Transport Coefficients, Oxygen, Nitrogen, Air.

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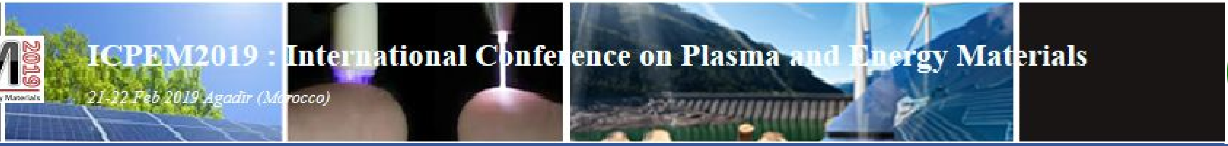

The Monte Carlo Simulation of Electron Transport Coefficients in Oxygen, Nitrogen, and Air

Mohammed Habib Allah Lahouel[1] ,Djilali Benyoucef[1, a] and Hocine Tebani[1]

[1] Laboratoire Génie Electrique et Energies Renouvelables, Chlef University, Algeria

[a)]d.benyoucef@univ-chlef.dz

Abstract

The main objective of this work is the calculation of the electron transport coefficients in oxygen, nitrogen, and air. They are calculated by using Monte Carlo method, and the results obtained are compared to the measurements in order to validate the used data for each gas.

Introduction

The electrical discharges in air are a technology of great interest for certain environmental-related industrial sectors such as water treatment and air sterilization by ozone generators or the depollution by precipitators, when it comes to the removal of industrial particles, dust and/or heavy metals; or by corona discharge reactors with or without DBD depending on the geometries of the electrodes [1,2,3]. The modeling makes it possible to optimize these electric discharges through the knowledge of the physical and chemical phenomena intervening in the discharge dynamic.

Generally the model used at atmospheric pressure is the fluid model, the latter is based on the first moments of the Boltzmann equation and requires some average quantities called transport coefficients.

Monte Carlo Method

The electron transport coefficients can be calculated by solving the Boltzmann equation:

$$\frac{\partial f}{\partial t} = \mathbf{v}.\nabla f - \frac{e}{m_e}\mathbf{E}.\nabla_v f = C[f]$$

This lat equation can be solved by using two different methods, the first one is the analytic method based on the development in Legendre polynomials [30], and the second one is the stochastic method called Monte Carlo Simulation Method [4,5,6,7,8] . This last is based on the processing of a sample of electrons and track their movements in the phase space, and this is done by integrating the equations of motion, taking into account the effect of the electromagnetic force applied on the electrons. In the case where an electron performs K kinds of collisions (elastic and inelastic collisions), The collision frequency $\upsilon(\varepsilon)$ is a function of the neutral density N, the total cross section $\sigma_T(\varepsilon)$, and the electron energy ε:

$$\upsilon(\varepsilon) = N.\sigma_T(\varepsilon).\sqrt{\frac{2\varepsilon}{m_e}}$$

where m_e is the electron mass. The collision probability $p(t_v)$ after a flight time t_v is given by:

$$1 - p(t_v) = 1 - \exp(-\int_0^{t_v} \upsilon_T(\varepsilon)dt)$$

$$\upsilon_{max} = N.\max\left\{\sum_{i=1}^{K} \sigma_i(\varepsilon).\sqrt{\frac{2\varepsilon}{m_e}}\right\}$$

$$t_{vol} = -\frac{\ln(1 - R_{vol})}{\upsilon_{max}}$$

where R_{vol} is a random number uniformly distributed between 0 and 1. The probability fraction of each type of collision (with υ_i frequency) is given by:

$$p_i = \frac{\upsilon_i}{\upsilon_{max}}$$

After each real collision, the scattering angles (axial χ and azimuthal ψ) is done by simple drawing of two random numbers (R_χ and R_ψ) distributed uniformly between 0 and 1, and in the case of an elastic collision, the electron energy loss is given by the following expression:

$$\Delta\varepsilon = 2\frac{m_e}{M}(1-\cos\chi)\varepsilon$$

$$\psi = 2\pi R_\psi \,,\, \chi = \mathrm{acos}(1 - 2R_\chi)$$

In the case of an inelastic collision, the electron energy reduces by a quantity correspond to the threshold energy of this collision, and in the case of the ionization an electron–ion pair is created, and the remainder energy will be divided between the ejected electron and the new electron. The electrons move under the effect of a uniform electric field applied in the opposite direction of the z-axis, and after a sufficient simulation time t_s, the electrons average energy stabilizes, and at this moment the transport coefficients can be evaluated by using the average values calculated from t_s to the final time of simulation t_f:

$$\mu_e = \frac{\langle z(t_f) - z(t_s)\rangle}{|E|(t_f - t_s)}, D_e = \frac{\left\langle (x(t_f)-x(t_s))^2 + (y(t_f)-y(t_s))^2\right\rangle}{4(t_f - t_s)}, \alpha = \frac{\ln\left(\left(\frac{n_0+\Delta n}{n_0}\right)+1\right)}{\langle z(t_f)-z(t_s)\rangle}$$

where n_0 and Δn are the electrons number at the time t_s and the electrons number variation from t_s to t_f respectively.

Results

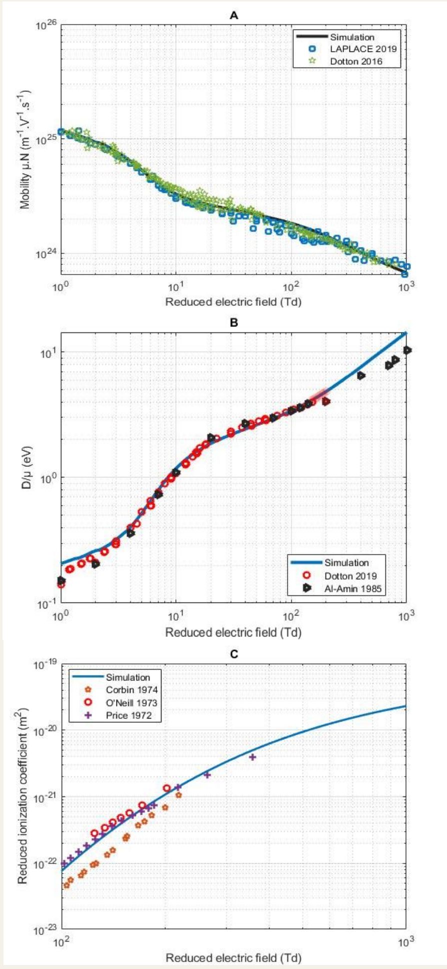

FIGURE 1. Comparison between the calculated and the measured transport coefficients of the electrons in Oxygen

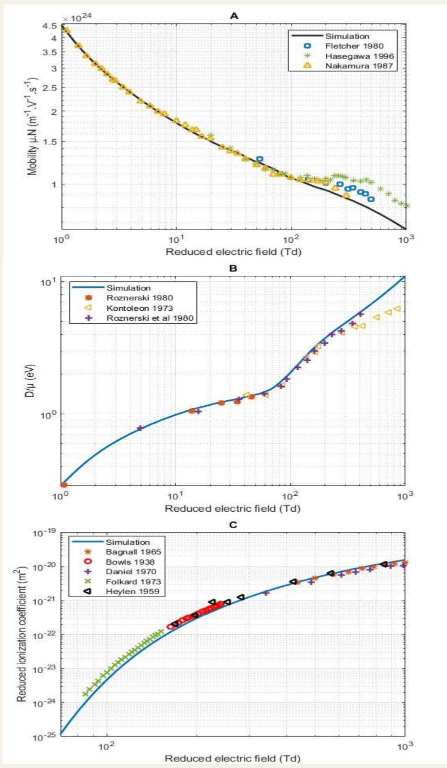

FIGURE 3. Comparison between the calculated and the measured transport coefficients of the electrons in Nitrogen

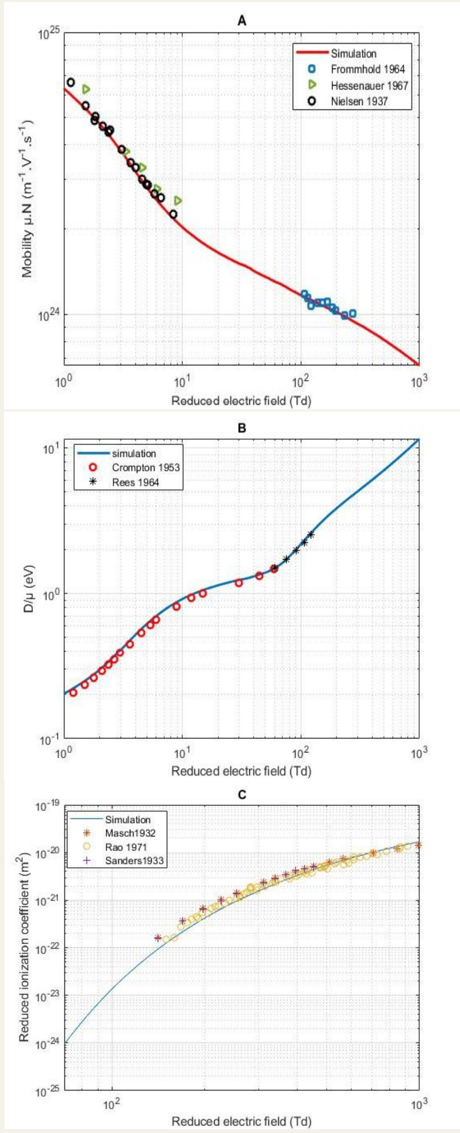

FIGURE 3. Comparison between the calculated and the measured transport coefficients of the electrons in dry Air

Conclusion

In this paper we have created a complete set of cross-sections for the different collision processes between the electron and the oxygen, Nitrogen and dry Air molecules; this set has been validated through the excellent reproduction of the electron transport coefficients. These latter are calculated by using Monte Carlo Simulation Method, which represents a very effective tool to solve the Boltzmann equation.

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Contact Information

Corresponding author's Name

Address: Laboratoire Génie Electrique et Energies Renouvelables, Chlef University, Algeria

Email:d.benyoucef@univ-chlef.dz

Web: www.univ-chlef.dz